The Barkas effect in crystal

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The contribution of the Barkas effect on the whole electronic stopping power is investigated via estimation of the maximum ranges of projectiles on channeling implantation. The screening effect due to target electrons on projectiles was essentially necessary for ions when they suffer almost maximum electronic stopping. A significant contribution of the Barkas effect on the maximum electronic ranges of ions was assured.

1. Introduction

Concerning with ion beam syntheses using high energy beam, preliminary estimation of maximum ranges, R_{max}, is an issue of the great consequence. In connection with this issue, it has been required to describe more accurately the dependence of the electronic stopping power, dE/dx, on the impact parameter, p, of implants [1]. Experiments with channeling have provided plenty of valuable information for this study.

Because of the different mechanisms of electronic stopping of target electrons for impinged ions with different ion velocities, the terms expressing dE/dx cannot be unique[2]: LSS theory[3] can give proper dE/dx making use of appropriate multiplying factor[4] for ions with low velocity, while Bethe-Bloch theory[5] is well accepted for ions with very high velocity. The description of dE/dx, for ions whose velocity is in an intermediate region where the maximum dE/dx is observed, is more complicated because of hybrid mechanism of electronic stopping.

There have been many trial formulae and theories to predict dE/dx, being available for ions with various velocity in a wide region. The significant contribution of higher Z_1 terms, being proportional to Z_1^3(Barkas term) and Z_1^4(Bloch term), was shown by Semrad et al.[6,7], where Z_1 expresses the atomic number of the projectile. They presumed uniform distribution of target electrons in principle. In order to describe the directional effect of dE/dx, which causes the different electronic ranges of channeled ions from those of random ones, we should take account the difference of local electron distribution observed by ions as they traverse along various trajectories. Therefore, reasonable expression including p-dependence of dE/dx has still been waited for ions in a rather wide velocity region, including specific velocity at which ions suffer maximum dE/dx. For this sake local density approximation (LDA) for dE/dx is the most promising approach.

Barkas et al.[8] found a difference in dE/dx between particles with same mass but opposite sign of charge, *e.g.* $\pi^+$and π^-, then it was regarded to be due to a term being propotional to the odd power of Z_1. L. H. Andersen et al.[9] also proved explicitly the contribution of this effect onto dE/dx, by means of excellent experiment with anti-proton.

Jackson and MacCathy[10] had ascribed this term to be only the distant collision and derived the Z_1^3term analytically. Ashlley et al.[11] derived this term with adopting a minimum impact parameter as an adjustable parameter. The latter provided a good agreement with experiments, while the former gave less dE/dx by a factor of two. Lindhard and Winther[12]had already stated the even contribution of close and distant collision to the total dE/dx (LW theory), and then Lindhard[13]explained satisfactory the Barkas effect observed from the difference in dE/dx for proton and antiproton. According to his expression the Barkas term increases with decreasing energy in proportional to $E^{-3/2}$. The velocity region for the plasmon excitation leading Barkas effect is confined. That is with increasing ion energy the bulk plasmon begins to be excited and then attenuated by absorption due to individual excitations (the Landau damping). Thus plasmon exists within meets two limiting ion energies.

The issue we discuss here is whether the screening due to target electrons is significant or not on the Barkas effect. Because the screening for the projectile should reduce the effective charge as ion velocity v decreases, while Barkas effect itself increases in proportional to v^{-3}. Various ions implanted into Si with an energy region of $20keV \leq E \leq 20MeV$ are concerned, especially paying attention to the influence of Barkas effect on dE/dx. Then we evaluate electronic ranges of axially channeled ions through crystalline Si, as one of the most trustable criteria.

2. Method

2.1 Electronic stopping power: dE/dx

The dE/dx is taken into account along each curved trajectory determined by the equation of motion, under the influence of surrounding atoms causing inelastic energy loss[14]. A crystal is represented as a bunch of axial channels, which is called cluster hereafter. The electron distribution in a cluster is depicted by a muffin-tin model[15]: The plausibility of muffin-tin model for a semiconductor of Si underlies experiments of plasmon absorption of this material, that is four of valence electrons per atom contribute to the volume plasmon of $\hbar\omega_p = 15eV$[16]. Inside each muffin of radius $r_{Muf} = 1.41A$, a spatial symmetric electron distribution[17] is adopted.

The dE/dx can be expanded in a series of Z_1 ; of those terms we discuss the second and third order contribution here, i.e., being proportional to Z_1^2(Bethe term) and Z_1^3(Barkas one). That is

$$\frac{dE}{dx}=\left(\frac{dE}{dx}(Z_1,Z_2,E,p)\right)_2+\left(\frac{dE}{dx}(Z_1,Z_2,E)\right)_3. \tag{1}$$

The first term is written[18]by as a product of $(Z_1\gamma)^2$and$(dE/dx)_p$for a proton moving through the electron gas of density $\rho(r)$ with energy E. The factor γ determining effective charge is much less than unity even when ions suffer the maximum dE/dx, *e. g.* $\gamma=0.92$ for B into Si with $30MeV$. Thus we adopt $Z_1\gamma$ instead of Z_1 even in the second term of eq. (1), *i.e.* ions are screened. For $(dE/dx)_p$we base on the LW theory, which can be expressed as a function both of energy E and local electron density $\rho(r)$ in solid [14,19]. As was stated by Mann and Brandt[20], however, LW is known to yield significantly small dE/dx for ions with lower velocity than the Fermi velocity of target electrons, so that we introduced a multiplying factor on it only in cases of low velocity ions. This is practically possible, if provided a bridge Scheme of dE/dx is adopted as will be shown in eq. (2). It could cover a wide energy region including intermidiate velocity region where the maximum dE/dx is observed. We express two asymptotic solutions of $(dE/dx)_p$ for high(S_H) and low (S_L) velocity ions, as functions of target electron density $\rho(A^{-3})$ and ion energy $E(keV/amu)$. That is, making use of a conventional way so far used[2,21],

$$\left(\frac{dE}{dx}\right)_p^{-1} = S_H^{-1}+(S_LC_L)^{-1}, \tag{2}$$

where C_L is a multiplying factor in order to compensate the lower dE/dx derived from LW theory. In the present article we employ $C_L = 2$ for all projectiles implanted into Si only for low energy ions. As for the second term Z_1^3term (Barkas effect), we follow the Lindhard expression.

2.2 Influence of Barkas effect on channeled ions

Electronic ranges are estimated by taking account the averaged dE/dx for channelled ions, $\langle dE/dx\rangle$, *i.e.*, integration of "$-\langle dE/dx\rangle^{-1}$"from the initial energy $E = E_o$ to a final energy $E = E_f$. Making use of $\langle dE/dx\rangle$ averaged over the whole cross section of a channel, the mean ranges, R_c, is given, as is compared with peak position of measured channel-peaks. On the other hand making use of $\langle dE/dx\rangle$ averaged over only the well-channeled ions, the maximum ranges, R_{max}, is given. Experimentally R_{max} is the depth where the member of 1/100 of projectiles embedded at R_c are observed in as-implanted materials[22]. The value E_f is determined from the channel fraction [15], which depends on the channel. For example, $E_f = 100eV$ for B into Si in ⟨100⟩ channel and $E_f = 14eV$ in ⟨100⟩ channel.

Here we discuss the case of channeling implantation of positively charged particles. Channeled ions preferentially moves nearby the center of axial channel where much less electrons distibute, therefore the contribution of valence electrons to the whole dE/dx for channeled ions is more important than that of core electrons. Because of the less dE/dx of valenee electros, this implies relatively the significance of the Barkas effect on channeling implantation. On the contrary when the dE/dx of core electrons is studied by means of negatively charged ions, we found that[23], the Barkas effect is of no importance for ions passing by the vicinity of nuclei. For example, 3 times larger dE/dx was obtained for antiprotons Channeling very closely to nuclei, as compared with random dE/dx for protons. For such amount of the difference in dE/dx the influence of the Barkas effect onto dE/dx of core electrons has no significance.

3. Results

3.1 Barkas effect for *H* into *Si*

Table 1 shows the calculated dE/dx of amorphous *Si* for protons in comparison with measured data or empirical values; data in the first column (Calc. 1) indicate the present result of dE/dx including the Barkas effect, while those in the last column (Calc. 2) show the dE/dx excluding it. The data denoted as"*SR*" is derived from an empirical formulae proposed by Semrad et al.[6], which is one of the most probable expression which agrees well not only with their precise experiments and also with other experiments, as well as TRIM by Biersack and Ziegler [24]and AZ by Andersen and Ziegler[2]. The contribution of the Barkas effect is significant especially around

E(keV)	Calc. 1	AZ	SR	TRIM	Calc. 2
20	5.057	8.725	9.618	8.728	5.057
40	6.653	11.10	11.88	11.65	6.653
60	7.430	12.07	12.27	12.98	7.430
80	9.221	12.26	12.00	13.34	7.793
100	12.60	12.03	11.51	13.15	7.933
200	11.19	9.574	9.082	10.35	7.506
400	7.388	6.784	6.530	7.053	6.103
600	5.723	5.484	5.291	5.586	5.118
800	4.776	4.678	5.543	4.714	4.435
1000	4.148	4.111	4.034	4.116	3.933
2000	2.650	2.630	2.783	2.631	2.602
4000	1.646	1.614	1.913	1.624	1.636
6000	1.227	1.197	1.532	1.209	1.223
8000	.9890	.9630	1.306	.9769	0.9868
10000	.8339	.8119	1.152	.8259	0.8326
20000	.4823	.4734	.7716	.4860	0.4820

Table 1 Values of dE/dx [eV/Å] for random proton implanted with energy E [keV] ; values indicated as Calc. 1 are the present calculation, those of Calc. 2 old one exculding Barkas effect [14], AZ by Andersen and Ziegler [2], SR by Semrad et al.[6], TRIM by Ziegler and Biersack[22].

maximum dE/dx.

3.2 Barkas effect for heavier ions

Table 2 shows the contribution of Z_1^{*3} terms to the whole dE/dx for ions with velocity at where TRIM predicts the maximum dE/dx. As is expected from the Z_1-dependence of the Barkas effect, it should be more remarkable for heavier ions with larger atomic numbers. Nevertheless polarization field introduced by an incident ion is reduced due to screening, which depends on the relative velocity of ion moving in solid. This apparent detailed balance should be discussed substantially from the viewpoint of localized plasmon. We presume here that the Barkas effect shall be described by Z_1^* not by Z_1. This difference is very distinct on discussing dE/dx around its maximum.

		H→Si (80keV)	He→Si (500keV)	B→Si (1.80MeV)
	γ	.96	.8	.55
$\frac{dE}{dx}$	Calc. 1 (eV/Å)	10	33	95
	Calc. 2 (eV/Å)	8	30	85
	TRIM (eV/Å)	13.34	35.99	101.00

Table 2 The significance of Z_1 values on the Barkas effect. $\gamma=$ (screened charge)/(bared charge), At the ion energy, given in parentheses, where TRIM calculation predicts the maximum dE/dx. Calc. 1 includes the Barkas effect whereas Calc. 2 neglects it.

3.3 R_{max} and R_c of B into Si

On evaluating the maximum ranges R_{max}, Barkas effect should be taken into account as extremely indispensable term. First reason is that this contributes to the whole dE/dx as weak as valence electrons, and second one is that the area of valence region is quite large as compared to core regions.

Calc. 1 in Table 3 shows the significance of Barkas effect on R_{max} of B into $Si\langle 100\rangle$ and $Si\langle 110\rangle$, as a case of heavy ion implantation. The influence on the channel peak (R_C) is not so significant. The calculated data ignoring Barkas effect are tabulated in columns denoted by Calc.2 for R_c[14] and R_{max}[15]. Experimental data are due to Kaim[25], Frey and Gong[26], and Rimini et al.[1,27].

4. Conclusions

In order to study the Barkas effect on the electronic stopping in solids, we evaluated dE/dx for ions, H, He, B, in amorphous Si and electronic ranges of B into $Si\langle 100\rangle$and $\langle 110\rangle$, in a ranges of intermediate velocity, $20keV \leq E < 20MeV$.

The heavier the projectile the more significance of the Barkas effect. We adopted the effective charge $Z_1^*$of projectiles not Z_1, *i.e.* projectiles are well screened as ion energy decreases. The contribution of the Barkas effect on the maximum ranges R_{max} on channeling implantation is more significant as compared to that on ranges R_c corresponding to channel peak in depth profiles. Maximum ranges of B into crystalline Si agreed well with measured data when Barkas effect was taken into account.

B-Si			R_C (Channel-peak) (μm)			R_{max} (Maximum range) (μm)		
Channel	E_0 (keV)	Ref.	Expt.	Calc. 1	Calc. 2	Expt.	Calc. 1	Calc. 2
<100>	10	25)	.13	.1927	.1927	.28	.2304	.2304
	20		.21	.2982	.2982	.41	.3539	.3539
	40		.3	.4482	.4482	.54	.5296	.5296
	80		.56	.6619	2.6619	.79	.7798	.7798
	80	1)	.52	.6619	.6619	.72	.7798	.7798
	150		.80	.9293	.9293	1.0	1.099	1.099
	200	26)	.877	1.083	1.083	1.2	1.284	1.284
	350	1)	1.25	1.451	1.451	1.6	1.742	1.742
	700		1.9	2.099	2.099	2.3	2.590	2.590
	990	26)	2.29	2.540	2.540	2.7	3.212	3.212
	2006		3.33	2.893	3.868	3.9	3.418	5.274
	3070		4.61	3.451	5.141	5.4	4.082	7.479
	6460		8.83	5.887	9.146	9.9	7.484	15.42
<110>	80	27)	.8	.8402	.8402	1.084	.8538	0.8538
	150		1.1	1.165	1.165	1.435	1.204	1.204
	350		1.72	1.781	1.781	2.094	1.921	1.921
	700		2.26	2.522	2.522	2.663	2.888	2.888

Table 3 Calc. 1 indicates the influence of the Barkas effect on electronic ranges, in comparison with the case obtained excluding this effect (Calc. 2).

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